JOURNAL OF MOLECULAR STRUCTURE, VOLUME 237 (1990)

AUTHOR INDEX

Abduljaber, M. 285
Aota, T. 105

Baran, J. 355
Barnes, A.J. 19
Bratek-Wiewiórowska, M.D. 123

Cambon, L. 411
Colemonts-Vandevyvere, C. 207
Czerminski, R. 151

de Kimpe, S.J. 339
Dore, J.C. 221

Ebata, T. 105
Efimov, Yu.Ya. 93
Etter, M.C. 165

Feil, D. 33
Finney, J.L. 249
Floersheim, P. 63

Graindourze, M. 389
Grootaers, T. 389
Guo, S. 307

Hadži, D. 139, 265
Huyskens, P. 207

Ito, M. 105

Janssen, L.H.M. 339
Jeffrey, G.A. 75

Kapuku, F. 207
Kidrič, J. 139, 265
Kleeberg, H. 187
Klein Kranenbarg, G.W. 339
Koller, J. 139
Kroon, J. 315
Kroon-Batenburg, L.M.J. 315
Kümmel, W. 233
Kwiatkowski, J.S. 151

Linschoten, M.R. 339
Luck, W.A.P. 233
Lutz, E.T.G. 355
Luu, D.V. 411

Maes, G. 389
Malinowska, N. 123
Marechal, Y. 273
Mathlouthi, M. 327, 411
Mavri, J. 139, 265
Mentel, T. 233
Mielke, Z. 273
Millen, D.J. 1

Person, W.B. 151
Plummer, P.L.M. 47
Podobnik, M. 265
Popenda, M. 123
Portmann, M.O. 327

Reutzel, S.M. 165

Scott, R.M. 285, 297, 307
Slanina, Z. 81
Smets, J. 389
Szczepaniak, K. 151

Tayh, J.A. 297
Tomkinson, J. 249

van der Maas, J.H. 355
van Eijck, B.P. 315
van Lenthe, J.H. 339
Videnova-Adrabinska, V. 367
Vojta, G.M. 165

Walkinshaw, M.D. 63
Wierzejewska Hnat, M. 355
Wiewiórowski, M. 123
Wilting, J. 339

Yamamoto, S. 105

Zeegers-Huyskens, Th. 389
Zelsmann, H.R. 273

JOURNAL OF MOLECULAR STRUCTURE, VOLUME 237 (1990)

SUBJECT INDEX

Acetic acids,
far IR spectra of acetic acids in the gas phase. A reinvestigation of the intermonomer vibrations 273
Acid malonates,
intramolecular hydrogen bonding in acid malonates. Infrared, NMR and ab initio MO investigations 265
Alcohols,
thermodynamics of H-bonding in alcohols and water. The mobile order theory as opposed to the classical multicomponent order theories 207
Ammonia,
studies of intermolecular interactions by matrix isolation vibrational spectroscopy: self-association of ammonia 19

n-Butylamine,
solvation of primary amines: short-range solvation of proton transfer complexes of 2,4-dinitrophenol and *n*-butylamine 307

Carbohydrates,
modelling OH···O hydrogen bonds in carbohydrates 75
CH_3CN,
spectroscopic investigation of ternary solutions: H_2O–CH_3CN–$Cu(ClO_4)_2$ 187
Computer modeling,
ensembles of hydrogen bonds in liquids, ice nuclei and in computer modeling 93
$Cu(ClO_4)_2$,
spectroscopic investigation of ternary solutions: H_2O–CH_3CN–$Cu(ClO_4)_2$ 187
dCyd hemiphosphate structure,
the nature of drastic differences in the recognition of protonated cytidinium and deoxycytidinium cations by their parent nucleosides within dihydrogenphosphate salts in the light of the computer-simulated crystal strucutre of dCyd hemiphosphate $(dCyd)_2H^+ H_2PO_4^-$ 123

Diethylamine,
stoichiometry of the short-range solvation of diethylamine in proton transfer reactions with 2,4-dinitrophenol and solvation by ethers 285
Dihydrogenphosphate salts,
the nature of drastic differences in the recognition of protonated cytidinium and deoxycytidinium cations by their parent nucleosides within dihydrogenphosphate salts in the light of the computer-simulated crystal strucuture of dCyd hemiphosphate $(dCyd)_2H^+H_2PO_4^-$ 123
Dimers,
the directional character of the hydrogen bond in gas-phase dimers 1
2,4-Dinitrophenol,
solvation of primary amines: short-range solvation of proton transfer complexes of 2,4-dinitrophenol and *n*-butylamine 307
2,4-Dinitrophenol,
stoichiometry of the short-range solvation of diethylamine in proton transfer reactions with 2,4-dinitrophenol and solvation by ethers 285
DNA,
hydrophilicity of proteins and DNA 63
Drug–receptor interactions,
the role of hydrogen bonding in drug–receptor interactions 139

Electron density distribution,
the electron density distribution in the hydrogen bond. A quantum chemical and crystallographic study 33
Ethers,
stoichiometry of the short-range solvation of diethylamine in proton transfer reactions with 2,4-dinitrophenol and solvation by ethers 285

5-Halogeno-uracils,
FT-IR spectroscopic study of uracil deriv-

atives and their hydrogen bonded complexes with proton donors. II. Monomer IR absorptions of thiouracils and 5-halogenouracils in argon matrices 389
H_2O,
spectroscopic investigation of ternary solutions: H_2O-CH_3CN-$Cu(ClO_4)_2$ 187
Hydrogen bond,
the directional character of the hydrogen bond in gas-phase dimers 1
Hydrogen bond,
the electron density distribution in the hydrogen bond. A quantum chemical and crystallographic study 33
Hydrogen bond,
molecular dynamics simulations and quantum mechanical studies of the hydrogen bond in water cluster systems 47
Hydrogen-bond complexes,
high-pressure and density dependence of H-bond complexes in solutions. A spectroscopic study of intermolecular interactions 233
Hydrogen bond ensembles,
ensembles of hydrogen bonds in liquids, ice nuclei, and in computer modeling 93
Hydrogen-bond networks,
hydrogen-bond networks in supercooled liquid water and amorphous/vitreous ices 221
Hydrogen-bonded organic compounds,
analysis of isotropic chemical shift data from high-resolution solid-state NMR studies of hydrogen-bonded organic compounds 165
Hydrogen bonding,
rotational isomerism, molecular motion and hydrogen bonding as studied by supersonic jet spectroscopy 105
Hydrogen bonding in alcohols and water,
thermodynamics of H-bonding in alcohols and water. The mobile order theory as opposed to the classical multicomponent order theories 207

Ices,
hydrogen-bond networks in supercooled liquid water and amorphous/vitreous ices 221
Ice nuclei,
ensembles of hydrogen bonds in liquids, ice nuclei and in computer modeling 93
ISIS,
ISIS: a new powerful tool for hydrogen bonding studies 249

Ligand-β-adrenoceptor complexes,
a computer modelling study of hydrogen bonds in ligand-β-adrenoceptor complexes: its implications in the deduction of a receptor map 339
Liquids,
ensembles of hydrogen bonds in liquids, ice nuclei and in computer modeling 93
Liquid-water structure,
perturbation of liquid-water structure by ionic substances 411

Molecular motion,
rotational isomerism, molecular motion and hydrogen bonding as studied by supersonic jet spectroscopy 105

$Na_3H(SO_4)_2$ single crystal,
polarized IR and Raman study of the $Na_3H(SO_4)_2$ single crystal 367
Nucleic acid bases,
intermolecular interactions and tautomerism of nucleic acid bases and their analogues 151

2-Phenyladamantan-2-ol,
polarized FTIR spectra of adamantanol derivatives. Part II. 2-Phenyladamantan-2-ol 355
Primary amines,
solvation of primary amines: short-range solvation of proton transfer complexes of 2,4-dinitrophenol and *n*-butylamine 307
Proteins,
hydrophilicity of proteins and DNA 63

Rotational isomerism,
rotational isomerism, molecular motion and hydrogen bonding as studied by supersonic jet spectroscopy 105

Secondary amines,
steric factors in the short-range solvation of secondary amines 297
Sugar molecules,
hydrogen-bond geometry around sugar

molecules: comparison of crystal statistics with simulated aqueous solutions 315
Supersonic jet spectroscopy,
rotational isomerism, molecular motion and hydrogen bonding as studied by supersonic jet spectroscopy 105
Sweet taste mechanism,
hydrogen bonding and the sweet taste mechanism 327

Ternary solutions,
spectroscopic investigation of ternary solutions: H_2O-CH_3CN-$Cu(ClO_4)_2$ 187
Thiouracils,
FT-IR spectroscopic study of uracil derivatives and their hydrogen bonded complexes with proton donors. II. Monomer IR absorptions of thiouracils and 5-halogenouracils in argon matrices 389

Water,
thermodynamics of H-bonding in alcohols and water. The mobile order theory as opposed to the classical mulitcomponent order theories 207
Water,
hydrogen-bond networks in supercooled liquid water and amorphous/vitreous ices 221
Water clusters,
computational studies of water clusters: temperature, pressure, and saturation effects on cluster fractions within the RRHO MCY-B/EPEN steam 81
Water cluster systems,
molecular dynamics simulations and quantum mechanical studies of the hydrogen bond in water cluster systems 47